Overview: ALPS/APEX Plasma Edge & Plasma Material Interaction Modeling Group

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Plasma Edge and Plasma/Material Interaction Modeling Group

Purpose

Undertake model integration and studies of the plasma edge and plasma/material interactions (PMI) that lead to:

1) fundamental understanding of the influences of plasma facing surfaces on fusion plasma performance

2) identifying performance limits and optimization strategies for advanced liquid and solid, first wall and PFC concepts.

Near Term Goal

Support the ALPS and APEX programs to help determine the feasibility of and optimization strategies for advanced first wall and PFC concepts.

Group Members

J. Brooks (ANL) – Chairman
JP. Allain (UIUC)
T. Evans (GA)
A. Hassanein (ANL)
S. Krasheninnikov (UCSD)
L. Owen (ORNL)
M. Rensink (LLNL)
T. Rognlien (LLNL)
D. Ruzic (UIUC)
C. Skinner (PPPL)
D. Stotler (PPPL)
R. Maingi (ORNL)
D. Whyte (UW)
C. Wong (GA)

Focus:

- DIII-D/DiMES-99 solid lithium shot analysis

- NSTX 1-m lithium module PMI analysis: erosion/redeposition, SOL transport, plasma performance.

- Liquid wall erosion/transport, temp. limits.

- Transient (ELM, VDE) liquid and solid surface response.

- Lithium PMI science: temp.-dependent sputtered angular and energy distributions, Li^+ sputtering and reflection (MD code analysis).

- Carbon and hydrocarbon erosion/transport, MD code reflection calculations. Mixed-material (Be/W) formation and sputtering (FIRE).

DiMES 99 Solid Lithium Shot Analysis

—Integrated sputtering/transport/redeposition analysis of 2/01 experiment.

—comparison with:
erosion data
lithium atom (Li I) photon data
lithium ion (Li II) photon data

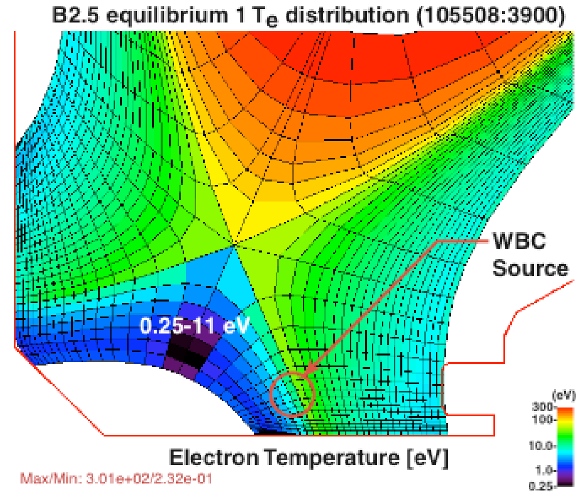
Allain, Brooks, Evans, Maingi, Owen, Finkenthal, Whyte, Wong

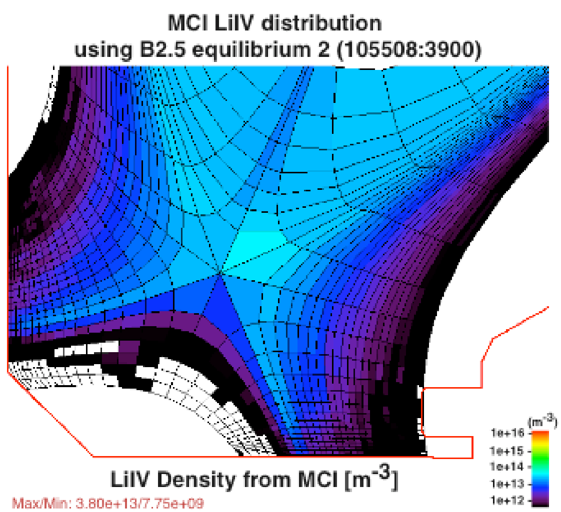
Lithium transport is being modeled in DIII-D with coupled fluid and kinetic codes

- Four specialized codes have been coupled to model Li sputtering and transport from a DIII-D DiMES sample
  - > background plasmas are simulated with the b2.5 / DEGAS fluid plasma / kinetic neutral deuterium code (L. Owen and R. Maingi at ORNL)
  - > Li sputtering sources are simulated with the gyro-kinetic WBC code (J. Brooks at ANL)
  - > Li transport is simulated by coupling the kinetic Monte Carlo Impurity (MCI) code to a b2.5 background plasma while using WBC Li sources (particle positions, velocities and charge states) as the initial conditions for the MCI simulation (T. Evans at GA and D. Finkenthal at Palomar)
- Initial comparisons of Li spectroscopic data from DIII-D discharge 105508 with MCI simulation results were inconclusive due to low Li concentration levels (below the 1% instrumental detection limit). Simulations predicted <1% and no emissions were observed.
- Additional Li DiMES experiments have been planned during 2003 that should provide good benchmarking data for the coupled simulations.

MCI/b2.5/DEGAS/WBC simulations result in a low Li core concentration for DIII-D shot 105508

- WBC uses D^+ flux from b2.5 and experimentally measured plasma parameters to calculate the sputtered Li distribution.
- MCI randomly samples 654 Li particle positions, charge states and velocities provided by WBC and follows them until they enter the inner core plasma at ψ_N = 0.92 or are lost to a plasma facing surface.





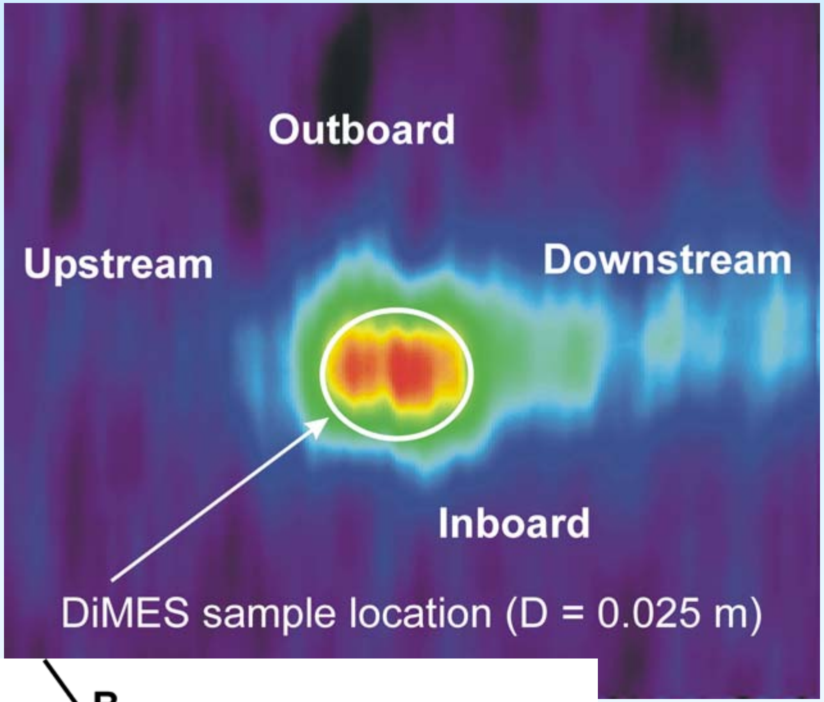
$R_{div\text{-}in} = R_{div\text{-}out} = 1.0$

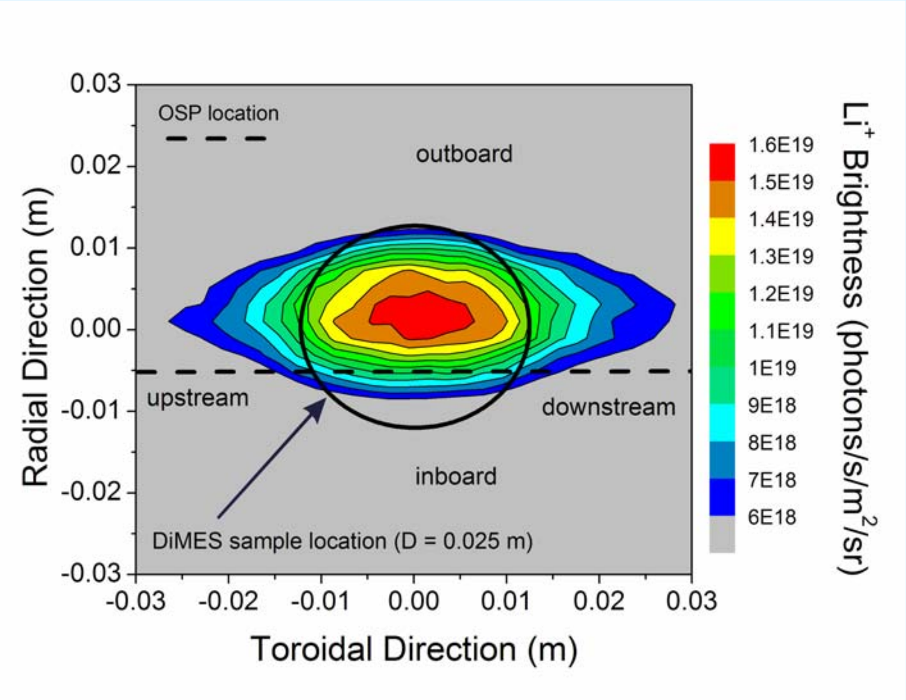
Core Li concentration ~ 0.0002% but is very sensitive to target plate recycling and private flux parameters

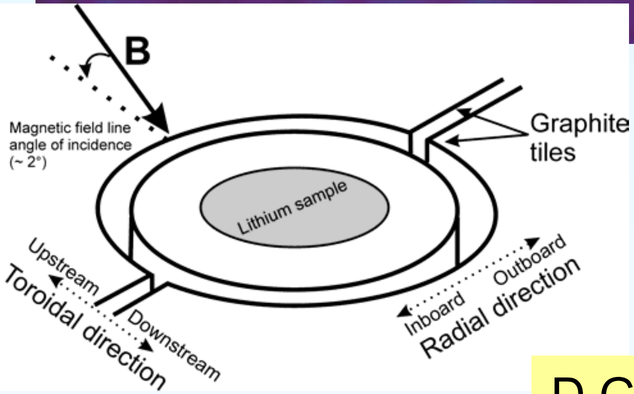
- Using b2.5 n_e and T_e, ASDS LiI->LiII rates and LiI velocities from WBC, we find neutral Li mean free path lengths (λ_{mfp}) above the sample of:
  > λ_{mfp} = 5.7 cm (inboard), λ_{mfp} = 1.8 cm (center) and λ_{mfp} = 0.4 cm (outboard)

  With a D^+ flux profile across the Li sample of:
  > 8.5e20 $m^{-2}\ s^{-1}$(inboard), 3.7e22 $m^{-2}\ s^{-1}$(center) and 3.9e21 $m^{-2}\ s^{-1}$(outboard).
- Stationary strike point experiments (105508 was swept) with heated Li will simplify the analysis.

Li-DiMES erosion modeling and measurements for solid-phase Li







Continued WBC/REDEP modeling of measured Li I and Li II light from Li-DiMES experiments under quiescent plasma conditions showing near-surface ionization of sputtered lithium

D.G. Whyte, J.N. Brooks and J.P. Allain

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Integrated NSTX lithium module erosion analysis

- Geometry: divertor module, ~ 8 cm poloidal by 100 cm toroidal.

- **2-D Plasma profiles: UEDGE Case sn_45; core power into the SOL = 6.0 MW ("low density/high-temp."). Peak heat load ~ 25 MW/m^2.**

- **Lithium surface temperature: SNL calculation for 10 m/s Li flow, UEDGE plasma heat load: T_s varies from 220 to 358 °C.**

- **D^+, Li^+ sputter yields: UIUC data/model, Y=Y(energy, species, T_s) for 45° incidence.**

- **Brooks/Allain et al. charged sputtered particle transport model, with MD calculations.**

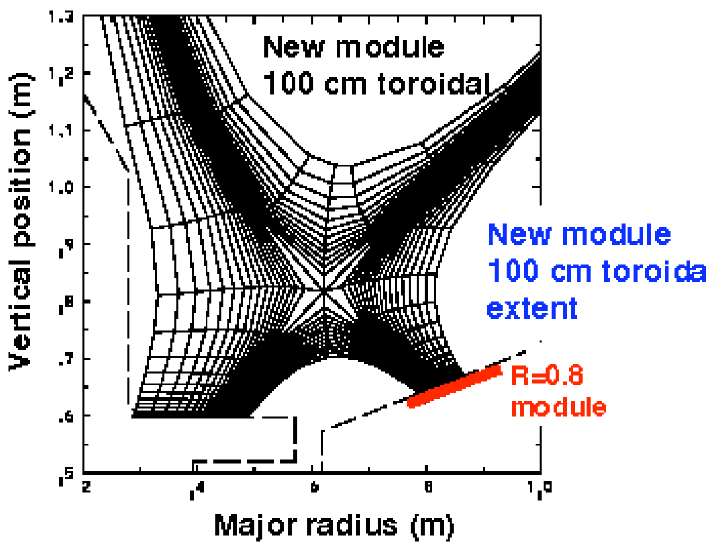
- **WBC calculation of self-consistent lithium sputtering from module, lithium flux to SOL, coupling to UEDGE.**

Edge plasma fluid modeling using UEDGE (Tom Rognlien and Marv Rensink, LLNL)

- **Edge-plasma characteristics for NSTX module**
  - Provide plasma for WBC near-sheath modeling
  - Use WBC lithium source to calculate influx to core
- **Highly radiating edge-plasmas for APEX CLIFF liquid-wall tokamak**
  - Allows high power removal from the scrape-off layer (SOL)
  - Stability, operating window, and core performance key issues
- **Impact of strong convective transport in far SOL**
  - Kotschenreuther's estimates show strong wall sputtering possible
  - Initial simulations indicate wall recycling is key to lower $T_{e,I}$ near the wall & thus sputtering

NSTX modeling extended to larger Li module

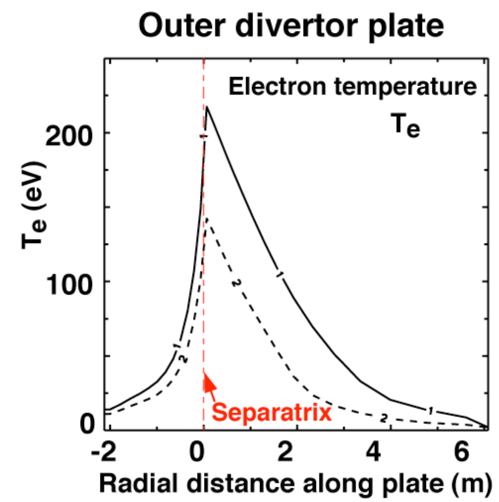
- **Module extended radially and toroidally**

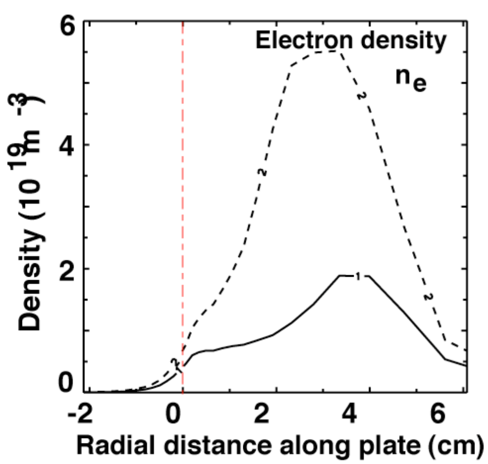


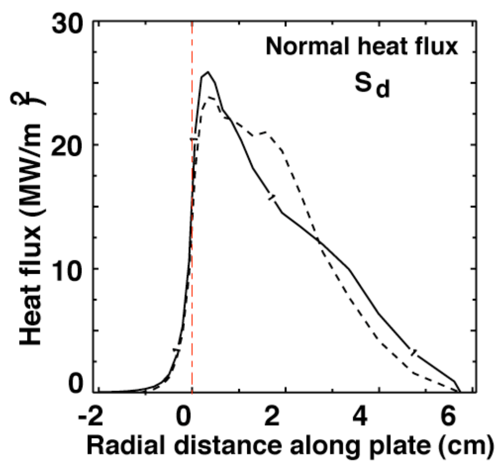
Legend

Present model of 1 m module pumping across entire outer plate; Reff = 0.8

Previous model for 0.4 m module pumping for R-Rsep > 2 cm, Reff = 0.9; for R-Rsep < 2 cm, Reff = 1.0

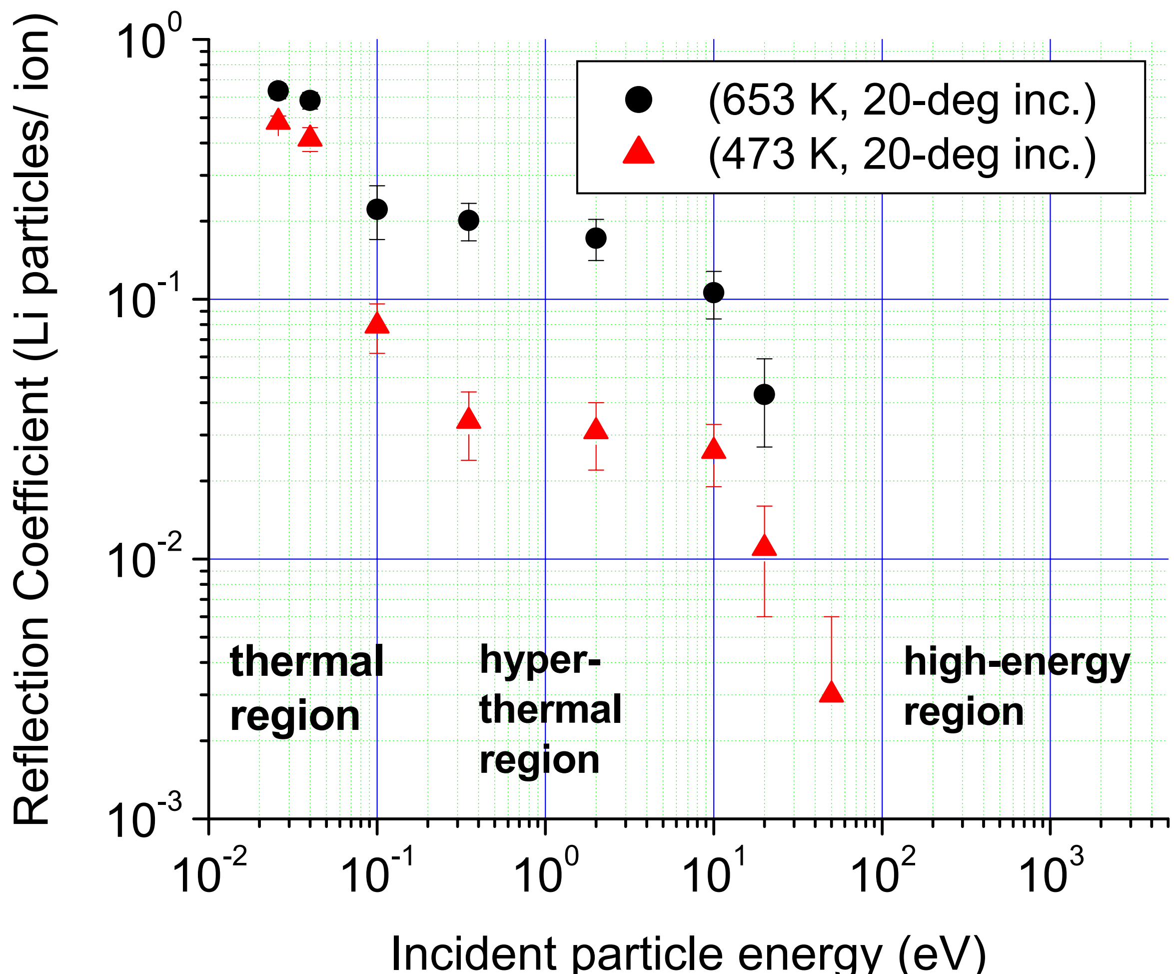






Molecular dynamics simulations of liquid lithium reflection

- NSTX cases: 473 and 653 K, 20-deg. incidence
- Reflection results show three distinct regions for low-energy self-bombardment reflection of lithium
- A region is found where the reflection coefficient varies little with incident energy (hyperthermal region)
- MD modeling continues to investigate this behavior as well as oblique bombardment (45,75-degree inc.)
- Other issues include: other temperatures and hydrogen treatment of lithium surface



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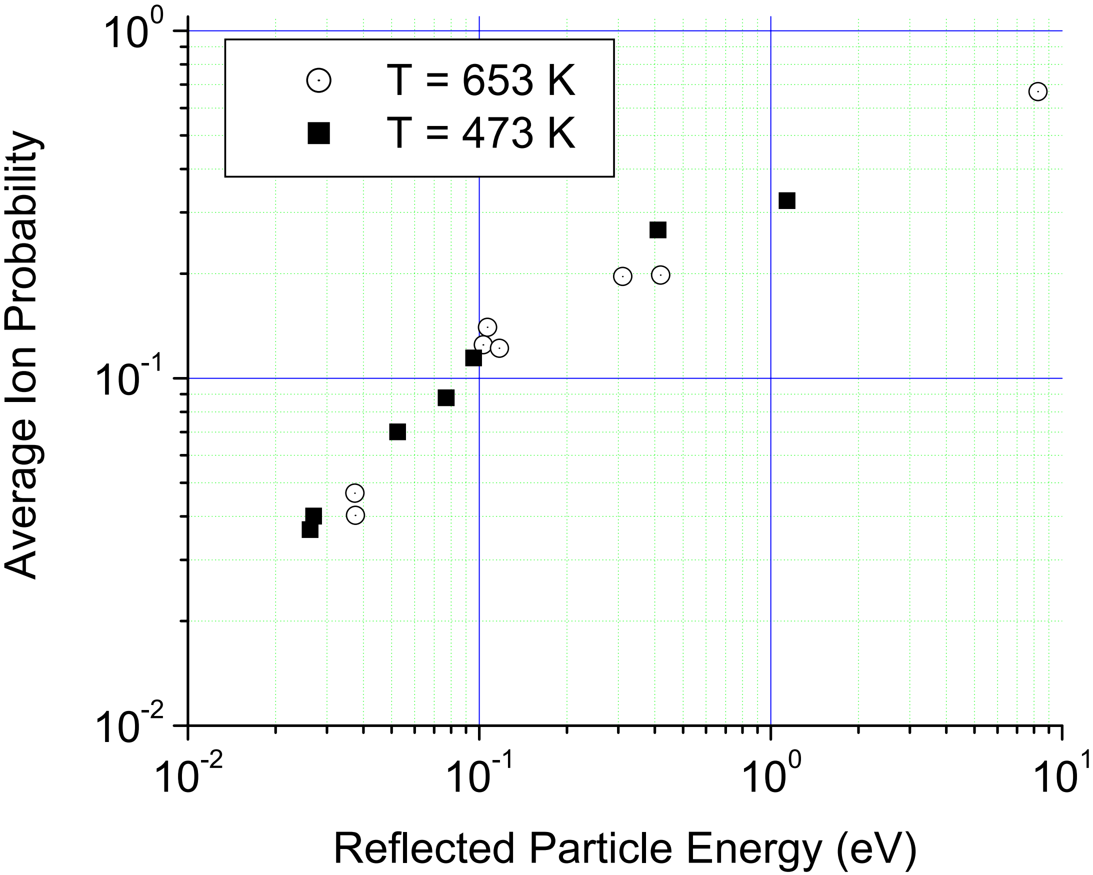
Ion probability of self-bombardment reflection from liquid Li surfaces

- Analytical model developed by R. Brako and D.M. Newns[1] for the charge state of backscattered alkali atoms from metals.
- At relatively low ($v_p < 10^3$ m/s) outgoing velocities and oblique emissions, alkali backscattered and ions are neutralized near the surface.
- The analytical model is coupled to MD calculations of the incident Li trajectory giving the outgoing velocities and elevation angle and resulting in the an average ion probability, P^+_{total}



$$P^+ = \exp\left[\frac{-2\Delta(z_c)}{\hbar \alpha v_p}\right]$$

$$P^+_{total} \equiv \sum_{N=1}^{100} \frac{P_N^+(v_p, \Theta)}{N}$$

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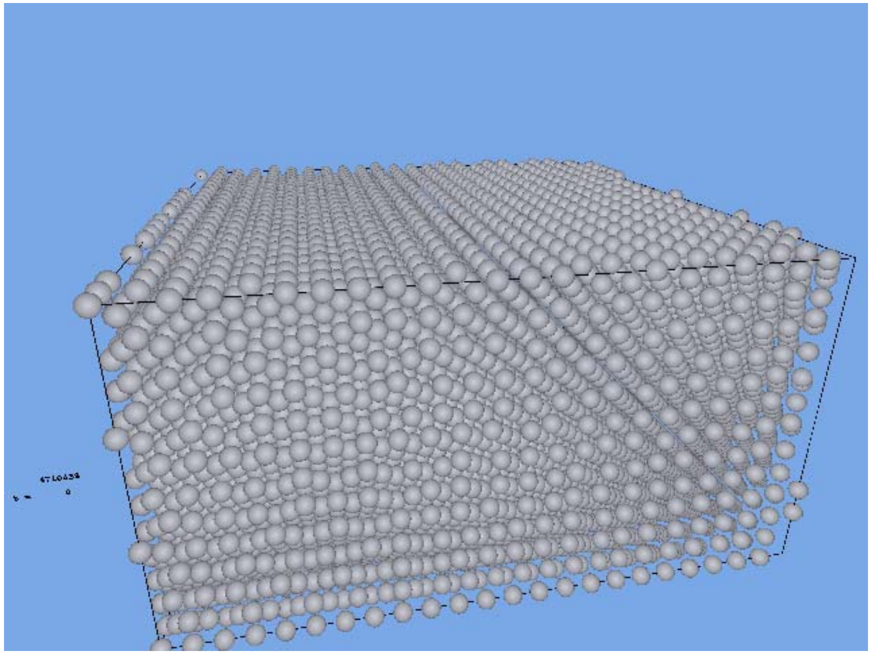
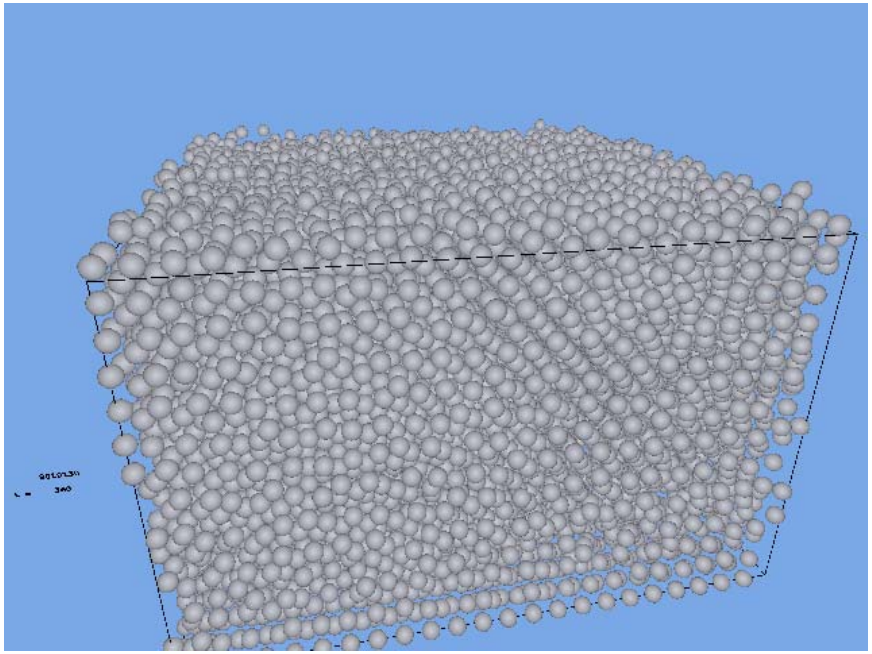
Analysis of molecular dynamics simulations of liquid surfaces





- Efforts begun in building larger lattices being mindful of computational expense.
- The size of the lattice may be relevant in modeling incident energies ranging from 100-700 eV. The effect of size on cascade dynamics are currently under investigation.
- A lithium lattice of about 13,300 lithium atoms is now in use and has been heated to temperatures of 473 and 653 K. Equilibration times ~ 250 picoseconds.

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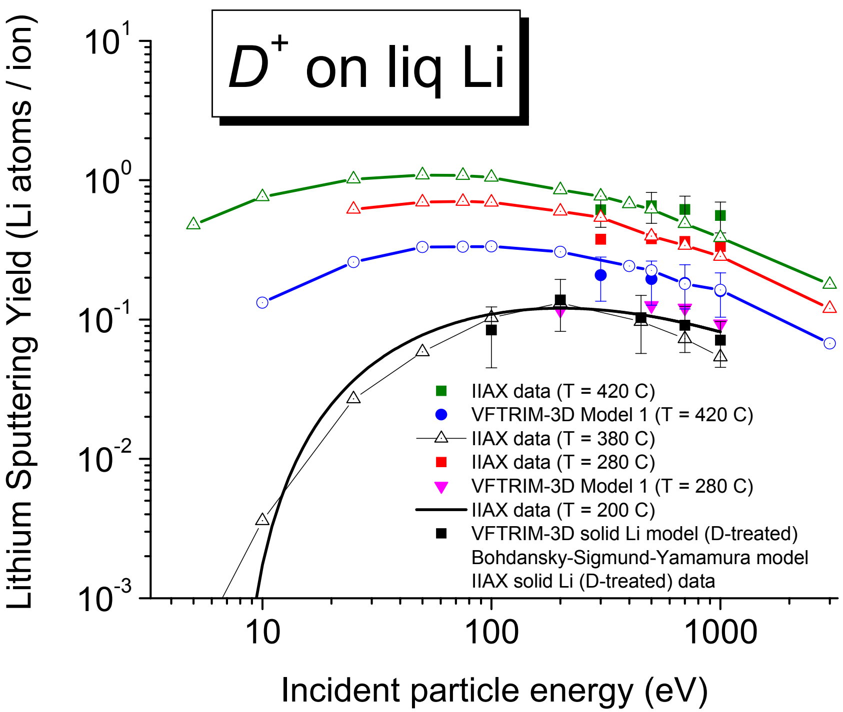
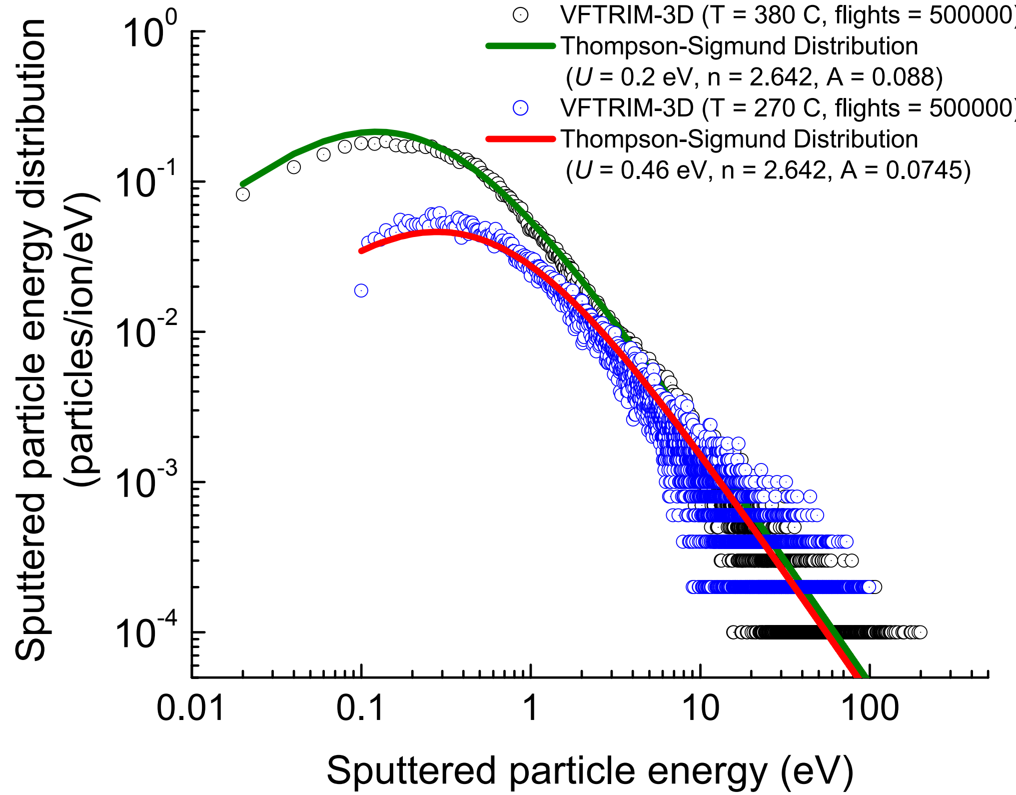
Temperature-dependent VFTRIM-3D energy and angular sputtered distributions for liquid Li†





- total sputtering yields showing maximum at lower incident particle energies
- VFTRIM-3D modeling with temperature-dependent submodels running 5 X 10^5 to 10^6 flights with NSTX cases: 270 and 380 °C, 20-degree incidence.

† The model in VFTRIM-3D will be upgraded with new model from molecular dynamics

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NSTX Lithium "one meter" module erosion; key REDEP/WBC Results

- ***Erosion/redeposition results are good.***

- **Self-sputtering yield peaks at ~ 0.4, i.e. much less than unity. Overall self-sputtering is finite (non-runaway).**

- **Overall lithium sputtering is high, but most lithium is confined to near-surface region, in spite of low plasma density.**

- **Sputtering superheat is moderate, ~ 1 MW/m^2**

- **Lithium current to SOL/near-surface boundary, ~ 4 % of sputtered current, is moderate.**

Progress on Assessment of NSTX Divertor Particle and Heat Fluxes (R. Maingi)

- NSTX is always (99%) in moderate-high recycling state and suffers from uncontrolled density rise
  - L-mode density increases with only NBI fueling
  - H-mode density increase > NBI fuel rate; τ_p^* ~ 0.2-0.4 sec

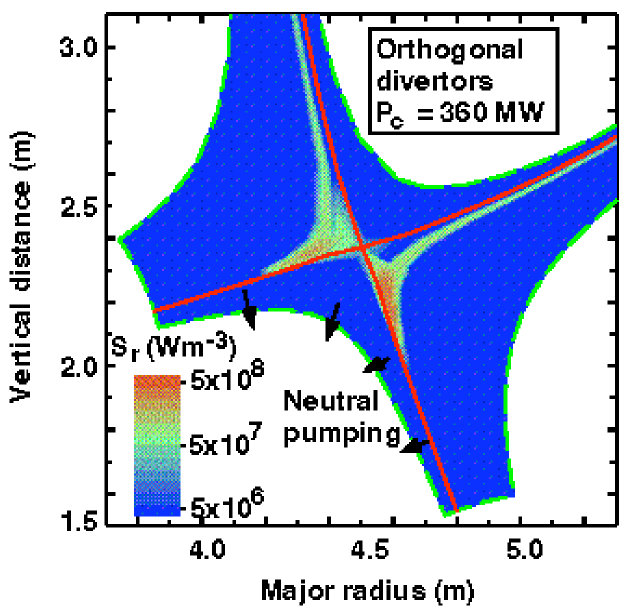
-> Density control needed, but where are particles and power?

- D_α peaks near inner and outer strike points, inner ~ 3x outer
  - Ratio reverses during power excursion -> inner probably detached
  - Most particles on outer side -> <u>consistent with module location</u>
- Heat flux always peaks near outer strike point
  - inner strike point peak heat flux and power < 1/3 outer values
  - > <u>consistent with module location</u>
- UEDGE modeling in progress; DEGAS-2/TRANSP to follow to estimate effect of lower recycling

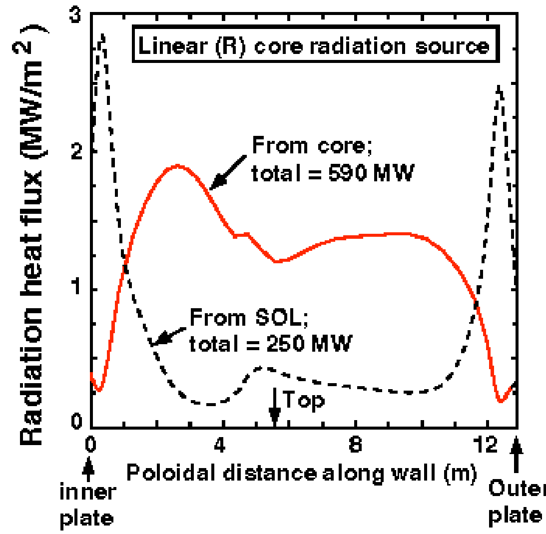
CLIFF wall with flinabe shows effective SOL radiation of core power if edge density ~ 1.5×10^{20}

- **Large SOL powers radiated by fluorine from flinabe wall**
- **Wall and divertor heat fluxes are acceptable**
- **Stability of detached divertor plasma is key issue**
- **Helium pumping needs assessment**

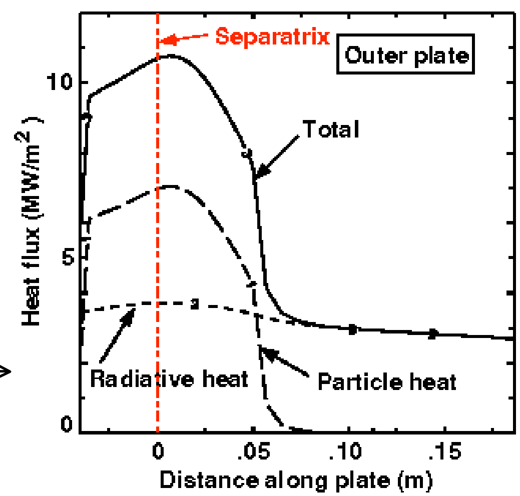
Fluorine radiation



Wall heat load



Divertor heat load



Rognlien
ALPS April '03

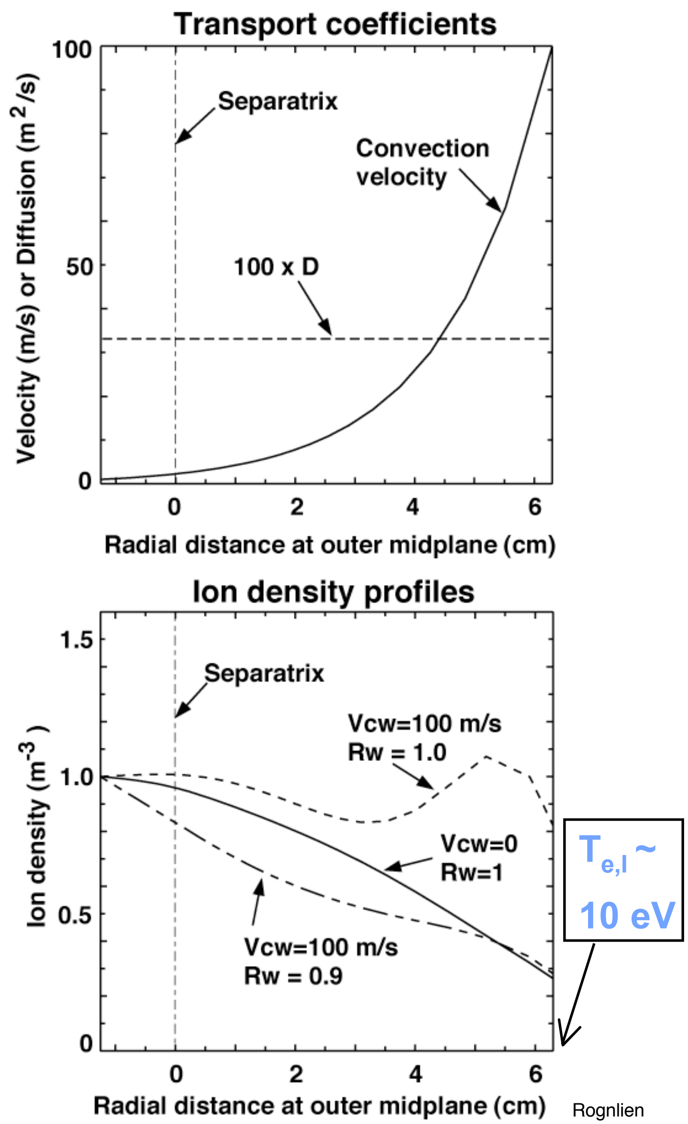
Plasma outward convection in the outer SOL may be a substantial source of wall sputtering

- Experimental data shows large transport in the far SOL
  ion flux = $-D\, d(n_i)/dr + n_i V_{conv}$

- Scaling from experiments, Kotschenreuther has found that such transport could give rise to significant first-wall sputtering

- Initial UEDGE modeling indicates that wall recycling is important in possibly reducing the plasma energy and thus sputtering

- High density and impurities help produce lower $T_{e,I}$ at the wall; much remains to be done



Rognlien
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HEIGHTS Simulations of Plasma/liquid Interactions (Hassanein et al. ANL)-recent ALPS Work

- **HEIGHTS package developed 3-D Molecular Dynamics (MD) capabilities to study important issues of plasma/liquid interactions**

- **MD simulation is now studying:**

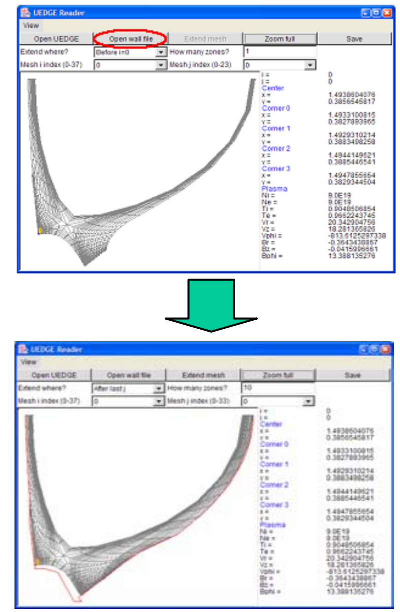
  - **He diffusion in liquid surfaces**
  - **H-isotope diffusion/retention in liquid surfaces**
  - **Mechanisms of enhanced liquid sputtering**
  - **He bubble formation dynamics and growth**

- **Preliminary simulation results show that He diffusion coefficient in liquid Lithium is in agreement with limited experimental data and theory. Self-diffusion and diffusion of other elements are in good agreement with available data.**

- **HEIGHTS continues to model plasma/liquid-solid interactions during various ELM regimes in different devices, particularly in QSPA and MK-200 Russian machines. Application analysis to NSTX etc continues.**

NSO/FIRE Modeling

- Original model
  - UEDGE plasma solution from Rognlien/Rensink was modified
    - Mesh extended out to first wall, plasma zones filled in
    - Modeled ion flux to first wall, including diffusive and anomalous transport
      - Flux = D x n_i / λ_n
      - $D_{perp} = D_{Bohm} = 0.06\ T_e/B$
      - $D_{anomalous} = 0.1\ m^2/s$ as in UEDGE
  - DEGAS2 used to calculate deuterium fluxes to first wall
  - Sputtering of beryllium from first wall calculated with VFTRIM-3D
  - Transport of sputtered Be to divertor calculated with WBC+
  - Results:
    - Be sputtering was low ($2.2 \times 10^{20}\ s^{-1}$)
    - Be current of $8.2 \times 10^{19}\ s^{-1}$ to inner and $2.9 \times 10^{19}\ s^{-1}$ to outer divertor plate



- Current flux model:
  - D_{perp} minimum is $0.1\ m^2/s$
  - Ion density at last UEDGE zone used (rather than at zone adjacent to wall)
  - Results:
    - Total Be sputtering increases to $4 \times 10^{20}\ s^{-1}$ (increased by about a factor of 2)
    - Be current of $1.8 \times 10^{20}\ s^{-1}$ (~ 2x) to inner and $8.4 \times 10^{19}\ s^{-1}$ (~3x) to outer divertor plate
- Beryllium flux to divertor goes to ANL for mixed material erosion analysis with the ITMC code

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CONCLUSIONS

- **DIII-DiMES solid lithium experiment under detailed, coupled, plasma material interaction analysis. Generally good code/data agreement seen (erosion, atom transport), with reasonable understanding of plasma/solid-lithium interaction.**

- **NSTX 1-m lithium divertor module under detailed analysis. From PMI standpoint, module could handle steady-state high power, and provide a high D pumping, low-recycle plasma.**

- **Major analytic results obtained on sputtered lithium ion transport. Molecular dynamic calculations show 2 eV Li^+ reflection coeff. ~ 0.1, with low reflected charge state.**

- **HEIGHTS code package analysis shows possibility of adequate helium pumping in flowing lithium, and surprising and encouraging preliminary results regarding ELM erosion mitigation by vapor clouds etc.**

- **Good progress on wall/plasma interactions, mixed material studies, and other PMI issues.**